



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 01:50 PM UTC

PDB ID : 2HAU / pdb_00002hau
Title : Apo-Human Serum Transferrin (Non-Glycosylated)
Authors : Wally, J.; Everse, S.J.
Deposited on : 2006-06-13
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

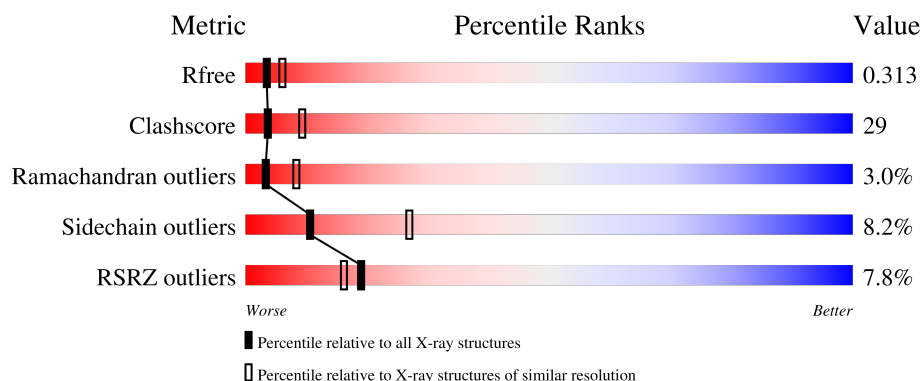
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	676	10% 47% 46% 6%
1	B	676	5% 49% 45% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10552 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

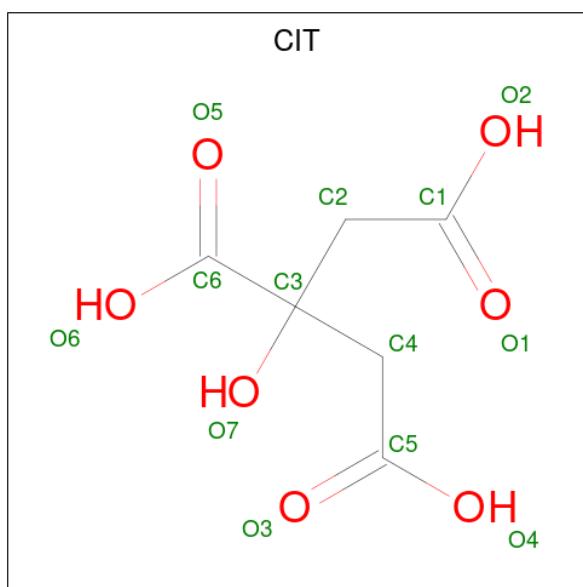
- Molecule 1 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	676	Total	C	N	O	S	Se	0	0	0
			5244	3291	907	999	38	9			
1	B	676	Total	C	N	O	S	Se	0	0	0
			5244	3291	907	999	38	9			

There are 22 discrepancies between the modelled and reference sequences:

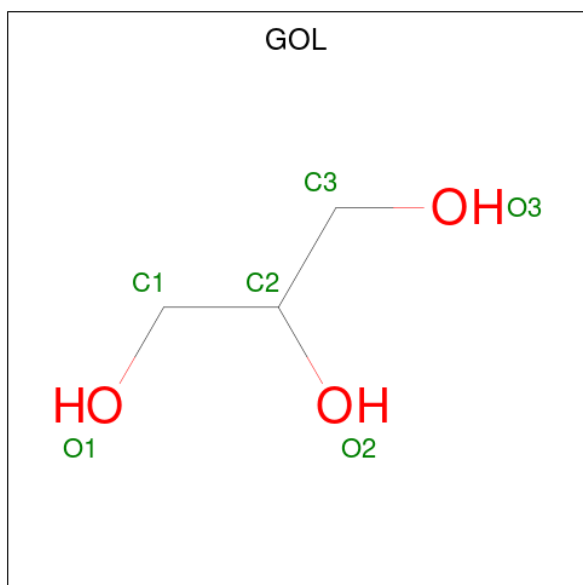
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MSE	MET	modified residue	UNP P02787
A	109	MSE	MET	modified residue	UNP P02787
A	256	MSE	MET	modified residue	UNP P02787
A	309	MSE	MET	modified residue	UNP P02787
A	313	MSE	MET	modified residue	UNP P02787
A	382	MSE	MET	modified residue	UNP P02787
A	389	MSE	MET	modified residue	UNP P02787
A	413	ASP	ASN	engineered mutation	UNP P02787
A	464	MSE	MET	modified residue	UNP P02787
A	499	MSE	MET	modified residue	UNP P02787
A	611	ASP	ASN	engineered mutation	UNP P02787
B	26	MSE	MET	modified residue	UNP P02787
B	109	MSE	MET	modified residue	UNP P02787
B	256	MSE	MET	modified residue	UNP P02787
B	309	MSE	MET	modified residue	UNP P02787
B	313	MSE	MET	modified residue	UNP P02787
B	382	MSE	MET	modified residue	UNP P02787
B	389	MSE	MET	modified residue	UNP P02787
B	413	ASP	ASN	engineered mutation	UNP P02787
B	464	MSE	MET	modified residue	UNP P02787
B	499	MSE	MET	modified residue	UNP P02787
B	611	ASP	ASN	engineered mutation	UNP P02787

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

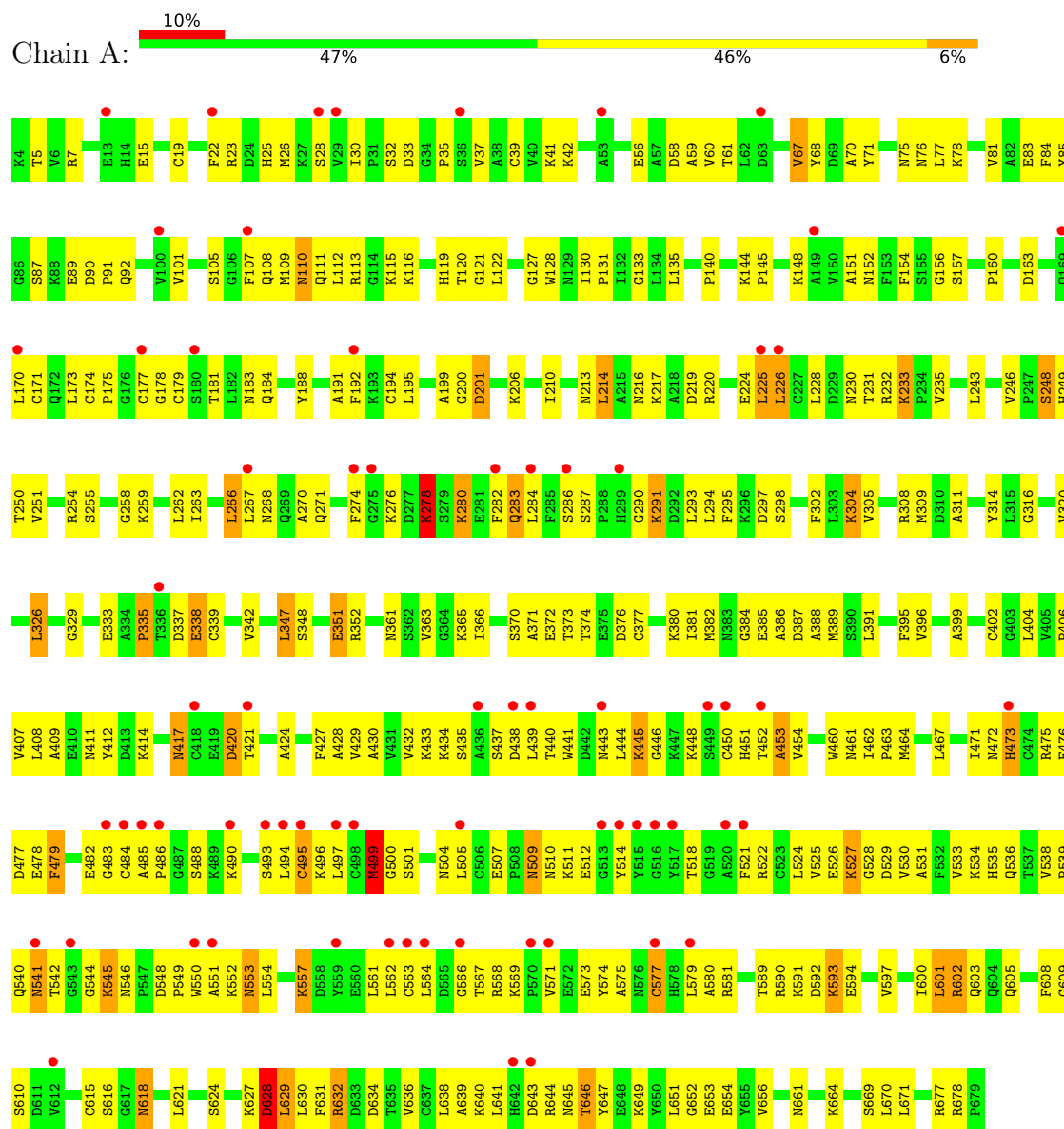


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots

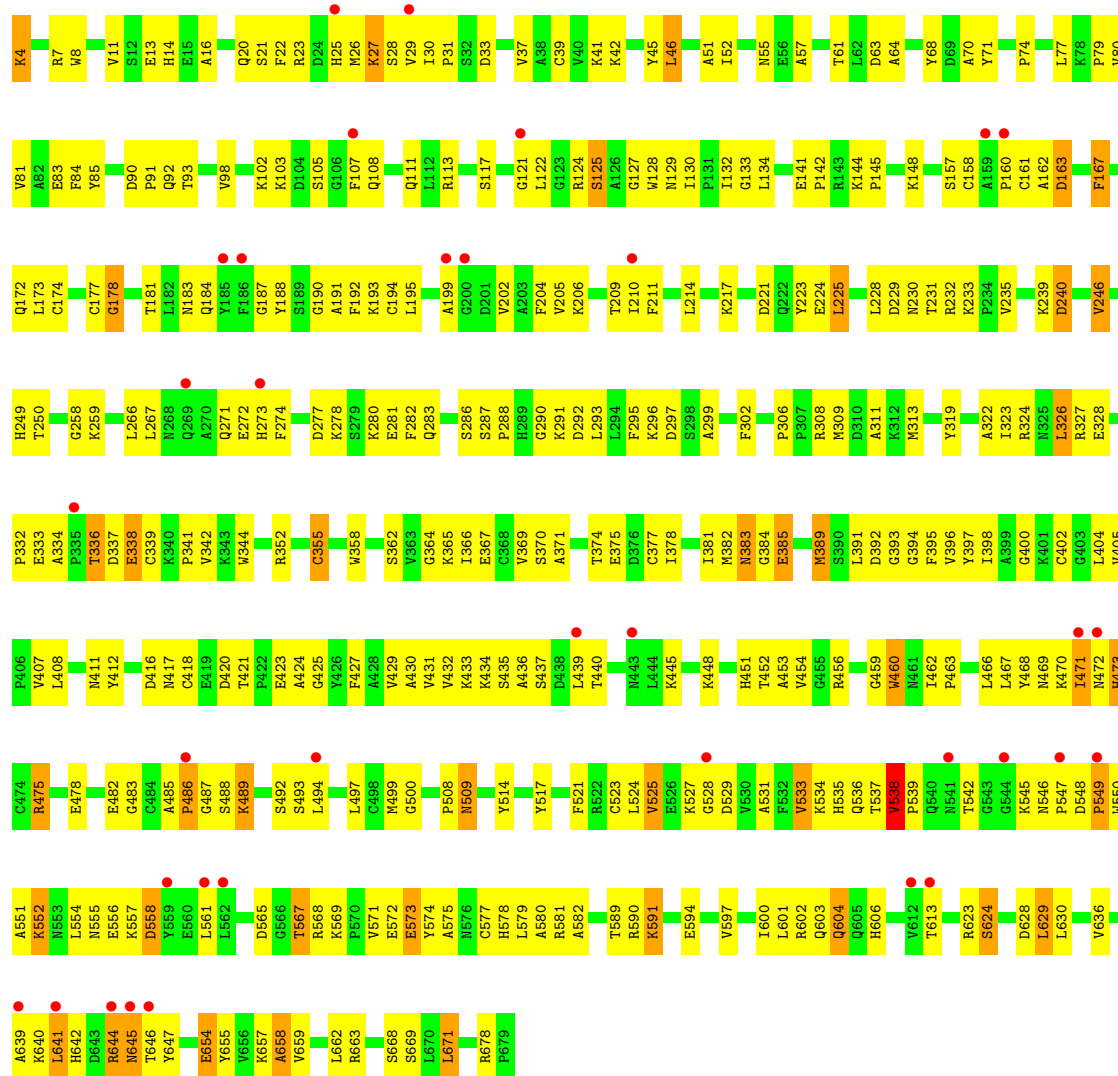
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Serotransferrin



• Molecule 1: Serotransferrin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.00Å 102.16Å 197.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.70) 93.3 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.324 0.279 , 0.313	Depositor DCC
R_{free} test set	2554 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10552	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.57	0/5354	0.98	12/7220 (0.2%)
1	B	0.60	2/5354 (0.0%)	0.98	10/7220 (0.1%)
All	All	0.59	2/10708 (0.0%)	0.98	22/14440 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	PRO	CA-C	5.36	1.57	1.52
1	B	538	VAL	CA-CB	5.07	1.57	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	658	ALA	N-CA-C	-7.11	101.37	110.19
1	A	384	GLY	N-CA-C	-6.87	105.58	114.85
1	B	396	VAL	N-CA-C	-6.80	103.68	110.62
1	B	306	PRO	CA-C-N	6.60	126.54	119.28
1	B	306	PRO	C-N-CA	6.60	126.54	119.28
1	A	652	GLY	N-CA-C	-6.50	105.00	112.29
1	B	355	CYS	N-CA-C	-6.15	104.57	111.28
1	B	167	PHE	CA-C-N	5.88	125.58	119.05
1	B	167	PHE	C-N-CA	5.88	125.58	119.05
1	B	63	ASP	N-CA-C	-5.78	103.30	110.41
1	A	68	TYR	N-CA-C	-5.48	105.38	111.36
1	A	396	VAL	N-CA-C	-5.47	105.19	110.72
1	A	479	PHE	N-CA-C	-5.47	106.66	113.55
1	A	248	SER	N-CA-C	5.46	117.99	111.71
1	A	56	GLU	N-CA-C	-5.26	106.71	113.23
1	B	202	VAL	N-CA-C	5.25	115.83	108.17
1	A	233	LYS	CA-C-N	5.16	125.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LYS	C-N-CA	5.16	125.16	119.90
1	A	250	THR	N-CA-C	5.15	117.82	109.06
1	A	67	VAL	N-CA-C	-5.08	105.59	110.72
1	A	280	LYS	N-CA-C	-5.06	107.14	113.72
1	B	385	GLU	N-CA-C	5.04	118.89	112.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5244	0	5064	313	0
1	B	5244	0	5064	291	0
2	A	13	0	5	1	0
2	B	39	0	15	1	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
All	All	10552	0	10164	602	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (602) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:THR:HG21	1:A:597:VAL:HG21	1.29	1.12
1:B:105:SER:HB2	1:B:232:ARG:HH22	1.19	1.04
1:B:624:SER:HB3	1:B:629:LEU:HG	1.40	1.03
1:A:602:ARG:HH11	1:A:602:ARG:HB2	1.19	1.02
1:A:538:VAL:HB	1:A:539:PRO:HD3	1.42	1.00
1:B:641:LEU:HB2	1:B:644:ARG:HB3	1.41	0.99
1:A:351:GLU:HG2	1:A:630:LEU:HD23	1.46	0.98
1:A:546:ASN:HD22	1:A:551:ALA:HB3	1.25	0.96
1:B:383:ASN:C	1:B:383:ASN:HD22	1.75	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:ASP:HB3	1:A:632:ARG:HA	1.52	0.89
1:A:551:ALA:HA	1:A:554:LEU:HD23	1.55	0.88
1:B:124:ARG:HH12	1:B:187:GLY:HA2	1.39	0.88
1:A:105:SER:HB2	1:A:232:ARG:HH22	1.39	0.88
1:A:351:GLU:HG2	1:A:630:LEU:CD2	2.04	0.87
1:B:309:MSE:HA	1:B:313:MSE:CE	2.05	0.87
1:A:15:GLU:HG2	1:A:294:LEU:CD1	2.05	0.86
1:B:668:SER:OG	1:B:671:LEU:HB2	1.73	0.86
1:A:15:GLU:HG2	1:A:294:LEU:HD13	1.58	0.85
1:A:23:ARG:HA	1:A:37:VAL:HG13	1.58	0.84
1:B:473:HIS:HB2	1:B:475:ARG:NE	1.92	0.84
1:A:420:ASP:HA	1:A:640:LYS:HE2	1.59	0.83
1:A:646:THR:OG1	1:A:649:LYS:HG2	1.79	0.83
1:B:108:GLN:H	1:B:111:GLN:HE21	1.27	0.82
1:B:538:VAL:HG13	1:B:539:PRO:HD3	1.61	0.82
1:B:27:LYS:HE3	1:B:27:LYS:HA	1.62	0.82
1:A:387:ASP:O	1:A:589:THR:HG22	1.81	0.81
1:B:29:VAL:HB	1:B:273:HIS:ND1	1.94	0.81
1:A:514:TYR:HE1	1:A:522:ARG:HG2	1.47	0.80
1:A:266:LEU:HD23	1:A:267:LEU:N	1.97	0.79
1:B:471:ILE:HB	1:B:473:HIS:CD2	2.18	0.79
1:A:308:ARG:HB2	1:A:669:SER:HB3	1.65	0.79
1:A:464:MSE:HE3	1:A:476:PHE:HB3	1.63	0.79
1:A:283:GLN:HB2	1:A:286:SER:HB3	1.64	0.79
1:A:484:CYS:HA	1:A:494:LEU:O	1.83	0.78
1:B:475:ARG:HD3	1:B:475:ARG:N	1.98	0.78
1:B:85:TYR:OH	1:B:296:LYS:HD2	1.84	0.77
1:A:602:ARG:HB2	1:A:602:ARG:NH1	1.97	0.77
1:B:383:ASN:C	1:B:383:ASN:ND2	2.39	0.77
1:B:383:ASN:ND2	1:B:385:GLU:H	1.83	0.77
1:A:70:ALA:HB1	1:A:77:LEU:HD12	1.65	0.77
1:A:434:LYS:HA	1:A:568:ARG:HH22	1.50	0.76
1:A:342:VAL:HG23	1:A:600:ILE:HD12	1.66	0.76
1:A:493:SER:HA	1:A:496:LYS:HE3	1.66	0.76
1:A:497:LEU:HD23	1:A:497:LEU:O	1.88	0.74
1:B:324:ARG:HD2	1:B:328:GLU:OE1	1.86	0.73
1:A:105:SER:HB2	1:A:232:ARG:NH2	2.04	0.73
1:B:488:SER:HB3	1:B:489:LYS:HE2	1.70	0.73
1:B:391:LEU:HD22	1:B:395:PHE:HB3	1.70	0.73
1:B:25:HIS:HB3	1:B:274:PHE:CZ	2.24	0.73
1:A:267:LEU:HD22	1:A:302:PHE:CE2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:SER:HB2	1:B:232:ARG:NH2	2.01	0.72
1:A:7:ARG:NE	1:A:58:ASP:OD1	2.19	0.72
1:A:432:VAL:HG12	1:A:530:VAL:HA	1.72	0.71
1:A:661:ASN:HA	1:A:664:LYS:HE3	1.72	0.71
1:B:124:ARG:NH1	1:B:187:GLY:HA2	2.05	0.71
1:A:427:PHE:H	1:A:535:HIS:HD2	1.39	0.71
1:B:362:SER:HB2	1:B:365:LYS:HB2	1.71	0.71
1:B:466:LEU:HD22	1:B:658:ALA:HB2	1.73	0.71
1:A:232:ARG:O	1:A:233:LYS:HG3	1.91	0.70
1:B:654:GLU:OE1	1:B:655:TYR:N	2.23	0.70
1:A:441:TRP:CZ2	1:A:467:LEU:HD13	2.27	0.70
1:B:287:SER:HB2	1:B:290:GLY:O	1.91	0.70
1:A:451:HIS:HD2	1:A:485:ALA:HB2	1.57	0.69
1:A:475:ARG:HD3	1:A:478:GLU:OE2	1.93	0.69
1:B:489:LYS:CE	1:B:489:LYS:H	2.06	0.69
1:B:561:LEU:HD12	1:B:571:VAL:HA	1.75	0.68
1:B:489:LYS:H	1:B:489:LYS:CD	2.06	0.68
1:A:557:LYS:HE2	1:A:557:LYS:HA	1.74	0.68
1:A:188:TYR:CZ	1:A:206:LYS:HE3	2.29	0.68
1:A:163:ASP:HB2	1:B:39:CYS:O	1.92	0.68
1:B:271:GLN:HE22	1:B:302:PHE:H	1.41	0.68
1:B:64:ALA:HB2	1:B:246:VAL:HG23	1.74	0.67
1:B:557:LYS:O	1:B:557:LYS:HD3	1.94	0.67
1:B:271:GLN:NE2	1:B:302:PHE:H	1.93	0.67
1:A:483:GLY:O	1:A:494:LEU:HA	1.95	0.67
1:B:429:VAL:HB	1:B:561:LEU:HD21	1.77	0.66
1:A:23:ARG:HA	1:A:37:VAL:CG1	2.25	0.66
1:A:22:PHE:HD2	1:A:37:VAL:HG21	1.60	0.66
1:B:641:LEU:CB	1:B:644:ARG:HB3	2.22	0.66
1:A:112:LEU:HD12	1:A:135:LEU:HD21	1.78	0.66
1:A:424:ALA:HB3	1:A:581:ARG:CZ	2.26	0.66
1:A:445:LYS:HD3	1:A:445:LYS:C	2.21	0.66
1:B:417:ASN:O	1:B:421:THR:HG22	1.95	0.66
1:A:429:VAL:HG21	1:A:561:LEU:HD13	1.78	0.66
1:B:61:THR:CG2	1:B:249:HIS:CD2	2.78	0.66
1:B:133:GLY:HA2	1:B:326:LEU:HD13	1.79	0.65
1:A:304:LYS:HG3	1:A:305:VAL:N	2.11	0.65
1:A:347:LEU:N	1:A:347:LEU:HD23	2.12	0.65
1:B:308:ARG:HB2	1:B:669:SER:HB3	1.79	0.65
1:B:535:HIS:CD2	1:B:536:GLN:HG2	2.32	0.65
1:A:440:THR:HG22	1:A:441:TRP:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:GLY:HA2	1:B:497:LEU:HD12	1.78	0.64
1:B:489:LYS:HE2	1:B:489:LYS:H	1.61	0.64
1:A:333:GLU:O	1:A:335:PRO:HD3	1.96	0.64
1:A:347:LEU:HD23	1:A:347:LEU:H	1.63	0.64
1:B:61:THR:HG21	1:B:249:HIS:CD2	2.32	0.64
1:A:521:PHE:O	1:A:525:VAL:HG23	1.97	0.64
1:B:470:LYS:O	1:B:471:ILE:HG23	1.98	0.64
1:B:107:PHE:HA	1:B:111:GLN:NE2	2.12	0.64
1:A:109:MSE:HE2	1:A:226:LEU:HB3	1.80	0.63
1:A:440:THR:HG22	1:A:441:TRP:N	2.13	0.63
1:A:116:LYS:HG2	1:A:173:LEU:HD11	1.80	0.63
1:B:542:THR:OG1	1:B:556:GLU:HG2	1.99	0.63
1:A:514:TYR:CE1	1:A:522:ARG:HG2	2.33	0.63
1:A:524:LEU:HD12	1:A:528:GLY:O	1.99	0.63
1:B:26:MSE:O	1:B:30:ILE:HG12	1.98	0.63
1:A:112:LEU:O	1:A:115:LYS:HB2	1.98	0.63
1:B:641:LEU:HD12	1:B:644:ARG:HB2	1.81	0.63
1:A:37:VAL:HB	1:A:266:LEU:HD11	1.81	0.62
1:A:509:ASN:N	1:A:509:ASN:HD22	1.96	0.62
1:B:7:ARG:HH22	1:B:55:ASN:ND2	1.96	0.62
1:A:216:ASN:HB2	1:A:219:ASP:OD2	2.00	0.62
1:A:538:VAL:HG11	1:A:571:VAL:HG21	1.81	0.62
1:B:240:ASP:OD1	1:B:678:ARG:NH2	2.32	0.62
1:B:429:VAL:HG12	1:B:578:HIS:HA	1.80	0.62
1:B:467:LEU:O	1:B:471:ILE:HG12	2.00	0.62
1:B:309:MSE:SE	1:B:313:MSE:HE3	2.50	0.62
1:B:473:HIS:HB2	1:B:475:ARG:CZ	2.29	0.61
1:A:179:CYS:H	1:B:20:GLN:HE22	1.49	0.61
1:B:229:ASP:OD1	1:B:231:THR:HB	2.00	0.61
1:B:267:LEU:HB3	1:B:302:PHE:CD2	2.35	0.61
1:B:408:LEU:HD23	1:B:640:LYS:HA	1.81	0.61
1:A:22:PHE:O	1:A:26:MSE:HG2	2.00	0.61
1:B:133:GLY:HA2	1:B:326:LEU:CD1	2.31	0.61
1:A:411:ASN:OD1	1:A:639:ALA:HB2	2.01	0.61
1:A:592:ASP:C	1:A:594:GLU:H	2.08	0.61
1:A:564:LEU:HD11	1:A:579:LEU:O	2.01	0.61
1:B:309:MSE:HA	1:B:313:MSE:HE2	1.81	0.60
1:B:375:GLU:OE1	1:B:668:SER:HB2	2.00	0.60
1:B:453:ALA:HB3	1:B:456:ARG:HG3	1.84	0.60
1:A:122:LEU:C	1:A:122:LEU:HD23	2.25	0.60
1:B:454:VAL:HG23	1:B:486:PRO:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:MSE:HE2	1:B:391:LEU:HD21	1.82	0.60
1:B:451:HIS:CD2	1:B:485:ALA:HB2	2.35	0.60
1:A:213:ASN:O	1:A:214:LEU:HD13	2.00	0.60
1:A:22:PHE:CD2	1:A:37:VAL:HG21	2.36	0.60
1:A:130:ILE:HB	1:A:131:PRO:HD3	1.83	0.60
1:B:29:VAL:HB	1:B:273:HIS:CE1	2.36	0.60
1:B:358:TRP:HE1	1:B:604:GLN:CG	2.15	0.59
1:B:489:LYS:HE2	1:B:489:LYS:N	2.17	0.59
1:B:462:ILE:HD13	1:B:580:ALA:HB3	1.82	0.59
1:A:195:LEU:HD12	1:A:200:GLY:O	2.02	0.59
1:A:624:SER:HB3	1:A:629:LEU:HG	1.84	0.59
1:A:267:LEU:HD22	1:A:302:PHE:CZ	2.37	0.59
1:A:451:HIS:CD2	1:A:485:ALA:HB2	2.38	0.59
1:A:409:ALA:HB2	1:A:641:LEU:HD21	1.84	0.59
1:A:488:SER:HB2	1:A:495:CYS:SG	2.43	0.59
1:B:210:ILE:HD13	1:B:235:VAL:HG11	1.85	0.59
1:B:124:ARG:HG2	2:B:9206:CIT:H22	1.84	0.59
1:B:141:GLU:HA	1:B:142:PRO:C	2.28	0.59
1:B:224:GLU:OE2	1:B:232:ARG:HD2	2.03	0.58
1:B:430:ALA:HB2	1:B:579:LEU:HD11	1.85	0.58
1:B:148:LYS:HB2	1:B:167:PHE:CE1	2.39	0.58
1:B:521:PHE:O	1:B:525:VAL:HG23	2.04	0.58
1:B:427:PHE:HB2	1:B:535:HIS:HB3	1.86	0.58
1:B:334:ALA:O	1:B:338:GLU:HB3	2.04	0.58
1:B:640:LYS:C	1:B:641:LEU:HD23	2.29	0.57
1:A:151:ALA:HB2	1:A:170:LEU:HD21	1.86	0.57
1:A:83:GLU:OE2	1:A:249:HIS:HD2	1.87	0.57
1:A:78:LYS:HG2	1:A:255:SER:HA	1.85	0.57
1:A:504:ASN:HA	1:A:507:GLU:HG3	1.85	0.57
1:B:424:ALA:HB3	1:B:581:ARG:CZ	2.35	0.57
1:B:468:TYR:C	1:B:470:LYS:H	2.13	0.57
1:B:425:GLY:HA3	1:B:582:ALA:O	2.04	0.57
1:A:25:HIS:CD2	1:A:282:PHE:HB2	2.39	0.57
1:B:602:ARG:NH2	1:B:640:LYS:HE2	2.20	0.57
1:A:231:THR:HG22	1:A:232:ARG:N	2.20	0.56
1:B:192:PHE:O	1:B:195:LEU:N	2.33	0.56
1:B:16:ALA:O	1:B:20:GLN:HG3	2.05	0.56
1:B:157:SER:HA	1:B:173:LEU:HD22	1.87	0.56
1:B:286:SER:O	1:B:288:PRO:HD3	2.06	0.56
1:B:641:LEU:HD12	1:B:644:ARG:CB	2.35	0.56
1:A:452:THR:O	1:A:453:ALA:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ALA:HA	1:A:486:PRO:HG2	1.86	0.56
1:A:440:THR:HG23	1:A:566:GLY:O	2.06	0.56
1:A:445:LYS:HD3	1:A:446:GLY:N	2.21	0.56
1:B:117:SER:O	1:B:157:SER:HB2	2.06	0.56
1:B:405:VAL:HG11	1:B:591:LYS:HD3	1.86	0.56
1:A:26:MSE:O	1:A:30:ILE:HB	2.06	0.56
1:B:158:CYS:O	1:B:160:PRO:HD3	2.06	0.56
1:B:391:LEU:HD22	1:B:395:PHE:CB	2.36	0.56
1:A:550:TRP:CZ3	1:A:551:ALA:HB2	2.41	0.56
1:B:514:TYR:CG	1:B:523:CYS:HB2	2.41	0.56
1:A:81:VAL:HG11	1:A:267:LEU:HD13	1.87	0.55
1:A:372:GLU:HG2	1:A:373:THR:HG23	1.88	0.55
1:A:471:ILE:HG22	1:A:473:HIS:O	2.06	0.55
1:B:514:TYR:CD2	1:B:523:CYS:HB2	2.42	0.55
1:A:568:ARG:O	1:A:569:LYS:HG3	2.07	0.55
1:B:27:LYS:HA	1:B:27:LYS:CE	2.36	0.55
1:A:605:GLN:OE1	1:A:638:LEU:N	2.36	0.55
1:B:640:LYS:HB2	1:B:644:ARG:HH12	1.71	0.55
1:A:81:VAL:HG21	1:A:267:LEU:HD12	1.88	0.55
1:A:110:ASN:N	1:A:110:ASN:HD22	2.05	0.54
1:A:119:HIS:HB3	1:A:127:GLY:O	2.07	0.54
1:A:546:ASN:ND2	1:A:548:ASP:HB2	2.21	0.54
1:B:471:ILE:HB	1:B:473:HIS:NE2	2.22	0.54
1:A:152:ASN:N	1:A:152:ASN:HD22	2.06	0.54
1:A:450:CYS:HB2	1:A:531:ALA:HA	1.89	0.54
1:B:27:LYS:NZ	1:B:30:ILE:HD11	2.21	0.54
1:B:291:LYS:HD2	1:B:297:ASP:OD2	2.06	0.54
1:B:80:VAL:HG23	1:B:81:VAL:HG23	1.90	0.54
1:B:23:ARG:HG3	1:B:37:VAL:O	2.08	0.54
1:A:181:THR:C	1:A:183:ASN:N	2.63	0.54
1:B:424:ALA:O	1:B:581:ARG:HG2	2.08	0.54
1:A:108:GLN:HB2	1:A:110:ASN:ND2	2.23	0.54
1:B:342:VAL:HB	1:B:366:ILE:HD13	1.90	0.54
1:B:641:LEU:HD23	1:B:641:LEU:N	2.22	0.54
1:B:68:TYR:CD2	1:B:323:ILE:HD13	2.43	0.54
1:B:383:ASN:HD22	1:B:384:GLY:N	2.06	0.54
1:B:418:CYS:HA	1:B:421:THR:CG2	2.38	0.54
1:A:105:SER:HB3	1:A:107:PHE:CE1	2.43	0.54
1:A:490:LYS:HE3	1:A:507:GLU:OE2	2.07	0.54
1:B:448:LYS:HB3	1:B:528:GLY:HA2	1.88	0.54
1:B:462:ILE:O	1:B:466:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:SER:HA	1:A:568:ARG:NH1	2.23	0.53
1:B:556:GLU:HB3	1:B:572:GLU:OE2	2.07	0.53
1:A:347:LEU:HD23	1:A:351:GLU:OE2	2.09	0.53
1:A:538:VAL:HB	1:A:539:PRO:CD	2.27	0.53
1:B:550:TRP:O	1:B:554:LEU:HD11	2.08	0.53
1:B:440:THR:HG22	1:B:568:ARG:HD2	1.89	0.53
1:A:280:LYS:NZ	1:A:280:LYS:HB3	2.24	0.53
1:A:471:ILE:O	1:A:473:HIS:N	2.42	0.53
1:A:154:PHE:O	1:A:156:GLY:N	2.41	0.53
1:B:411:ASN:ND2	1:B:639:ALA:HB2	2.24	0.53
1:B:555:ASN:O	1:B:558:ASP:HB2	2.08	0.53
1:A:427:PHE:H	1:A:535:HIS:CD2	2.23	0.53
1:A:509:ASN:HD22	1:A:509:ASN:H	1.57	0.53
1:A:552:LYS:HG2	1:A:553:ASN:CG	2.34	0.53
1:B:658:ALA:O	1:B:659:VAL:HB	2.09	0.53
1:B:333:GLU:HG2	1:B:334:ALA:N	2.24	0.52
1:B:437:SER:HA	1:B:568:ARG:NH1	2.23	0.52
1:B:378:ILE:HG23	1:B:404:LEU:HD22	1.91	0.52
1:B:475:ARG:HG3	1:B:478:GLU:OE2	2.09	0.52
1:A:534:LYS:CE	1:A:536:GLN:HE21	2.23	0.52
1:B:8:TRP:HH2	1:B:267:LEU:HD11	1.74	0.52
1:B:283:GLN:HB2	1:B:286:SER:HB3	1.91	0.52
1:B:551:ALA:HA	1:B:554:LEU:CD1	2.39	0.52
1:A:144:LYS:HA	1:A:145:PRO:C	2.34	0.52
1:A:542:THR:O	1:A:545:LYS:HE3	2.10	0.52
1:B:191:ALA:O	1:B:194:CYS:HB3	2.10	0.52
1:A:268:ASN:C	1:A:270:ALA:H	2.16	0.52
1:A:433:LYS:C	1:A:435:SER:H	2.17	0.52
1:A:151:ALA:HB2	1:A:170:LEU:CD2	2.39	0.52
1:B:108:GLN:N	1:B:111:GLN:HE21	2.02	0.52
1:B:228:LEU:C	1:B:230:ASN:H	2.17	0.52
1:B:466:LEU:CD2	1:B:658:ALA:HB2	2.39	0.52
1:B:597:VAL:O	1:B:601:LEU:HB2	2.10	0.52
1:A:414:LYS:C	1:A:414:LYS:HD2	2.35	0.52
1:B:188:TYR:OH	1:B:206:LYS:HG3	2.10	0.52
1:B:249:HIS:ND1	1:B:296:LYS:HE2	2.25	0.52
1:B:524:LEU:HB2	1:B:531:ALA:HB2	1.92	0.52
1:A:380:LYS:HG2	1:A:385:GLU:HB2	1.92	0.52
1:B:473:HIS:HB2	1:B:475:ARG:HE	1.72	0.52
1:B:22:PHE:O	1:B:26:MSE:HG2	2.09	0.51
1:B:407:VAL:HG21	1:B:597:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HG2	1:A:42:LYS:N	2.24	0.51
1:A:113:ARG:HG2	1:A:113:ARG:HH11	1.76	0.51
1:B:102:LYS:O	1:B:105:SER:OG	2.28	0.51
1:B:535:HIS:CD2	1:B:536:GLN:H	2.28	0.51
1:B:117:SER:OG	1:B:157:SER:CB	2.59	0.51
1:B:309:MSE:HA	1:B:313:MSE:HE3	1.87	0.51
1:A:592:ASP:O	1:A:594:GLU:N	2.44	0.51
1:A:192:PHE:CZ	1:A:210:ILE:HG13	2.46	0.51
1:A:148:LYS:O	1:A:151:ALA:HB3	2.10	0.51
1:A:225:LEU:HD13	1:A:235:VAL:HG12	1.93	0.51
1:A:605:GLN:CD	1:A:638:LEU:H	2.19	0.51
1:A:108:GLN:HA	1:A:226:LEU:HD21	1.93	0.50
1:B:61:THR:HG22	1:B:249:HIS:CD2	2.45	0.50
1:A:592:ASP:C	1:A:594:GLU:N	2.69	0.50
1:B:144:LYS:HA	1:B:145:PRO:C	2.36	0.50
1:B:91:PRO:O	1:B:92:GLN:HB2	2.10	0.50
1:B:323:ILE:HG12	1:B:327:ARG:HD3	1.94	0.50
1:A:267:LEU:HB3	1:A:302:PHE:CD2	2.46	0.50
1:A:290:GLY:C	1:A:291:LYS:HD2	2.36	0.50
1:B:188:TYR:HB3	1:B:209:THR:HG23	1.94	0.50
1:A:171:CYS:O	1:A:174:CYS:C	2.55	0.50
1:A:225:LEU:HD22	1:A:235:VAL:HA	1.93	0.50
1:B:668:SER:HG	1:B:671:LEU:HB2	1.74	0.50
1:A:352:ARG:HD3	1:A:370:SER:OG	2.11	0.50
1:B:565:ASP:OD2	1:B:567:THR:HG23	2.11	0.50
1:B:641:LEU:O	1:B:642:HIS:C	2.54	0.50
1:B:70:ALA:HB1	1:B:77:LEU:HD12	1.94	0.50
1:B:283:GLN:OE1	1:B:283:GLN:N	2.45	0.50
1:A:441:TRP:CE2	1:A:467:LEU:HD13	2.47	0.49
1:B:509:ASN:N	1:B:509:ASN:HD22	2.11	0.49
1:B:129:ASN:O	1:B:133:GLY:N	2.45	0.49
1:B:482:GLU:HA	1:B:493:SER:HB2	1.94	0.49
1:B:534:LYS:HE3	1:B:536:GLN:HG3	1.94	0.49
1:B:551:ALA:HA	1:B:554:LEU:HD12	1.94	0.49
1:A:109:MSE:H	1:A:226:LEU:HD22	1.77	0.49
1:A:534:LYS:HE3	1:A:536:GLN:HE21	1.78	0.49
1:B:439:LEU:HD21	1:B:529:ASP:HB3	1.95	0.49
1:A:550:TRP:CE3	1:A:551:ALA:HB2	2.48	0.49
1:B:117:SER:OG	1:B:157:SER:HB3	2.12	0.49
1:A:259:LYS:O	1:A:263:ILE:HG13	2.11	0.49
1:A:109:MSE:CE	1:A:226:LEU:HB3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:TRP:CZ3	1:B:267:LEU:HD21	2.47	0.49
1:B:468:TYR:O	1:B:470:LYS:N	2.46	0.49
1:B:641:LEU:H	1:B:644:ARG:NH1	2.11	0.49
1:A:112:LEU:O	1:A:113:ARG:C	2.55	0.49
1:A:387:ASP:OD1	1:A:593:LYS:HE2	2.13	0.49
1:B:535:HIS:CD2	1:B:536:GLN:N	2.80	0.49
1:A:37:VAL:HB	1:A:266:LEU:CD1	2.42	0.49
1:B:121:GLY:HA2	1:B:160:PRO:HB2	1.95	0.49
1:A:451:HIS:O	1:A:486:PRO:HD2	2.13	0.48
1:A:590:ARG:O	1:A:592:ASP:O	2.30	0.48
1:B:468:TYR:C	1:B:470:LYS:N	2.68	0.48
1:B:499:MSE:HG3	1:B:500:GLY:N	2.28	0.48
1:A:181:THR:C	1:A:183:ASN:H	2.19	0.48
1:B:383:ASN:HD21	1:B:385:GLU:HB2	1.77	0.48
1:A:15:GLU:HG2	1:A:294:LEU:HD12	1.92	0.48
1:B:177:CYS:O	1:B:178:GLY:C	2.56	0.48
1:B:352:ARG:HD3	1:B:370:SER:OG	2.13	0.48
1:B:451:HIS:HD2	1:B:485:ALA:HB2	1.77	0.48
1:A:365:LYS:HE2	1:A:603:GLN:NE2	2.28	0.48
1:A:108:GLN:H	1:A:111:GLN:HG3	1.78	0.48
1:B:431:VAL:HG13	1:B:524:LEU:HD22	1.95	0.48
1:A:562:LEU:HD23	1:A:563:CYS:N	2.28	0.48
1:A:589:THR:CG2	1:A:597:VAL:HG21	2.21	0.48
1:B:70:ALA:HB1	1:B:77:LEU:HB2	1.95	0.48
1:B:214:LEU:HD11	1:B:223:TYR:HE2	1.79	0.48
1:A:120:THR:OG1	1:A:127:GLY:HA3	2.13	0.48
1:A:157:SER:N	1:A:173:LEU:HD13	2.29	0.48
1:A:483:GLY:N	1:A:497:LEU:HD13	2.28	0.48
1:B:341:PRO:HB3	1:B:364:GLY:O	2.14	0.48
1:A:157:SER:CA	1:A:173:LEU:HD13	2.44	0.48
1:A:291:LYS:HG3	1:A:297:ASP:OD1	2.14	0.48
1:A:347:LEU:CD2	1:A:351:GLU:OE2	2.62	0.48
1:B:358:TRP:HE1	1:B:604:GLN:HG2	1.78	0.48
1:A:283:GLN:CB	1:A:286:SER:HB3	2.39	0.47
1:A:417:ASN:O	1:A:421:THR:HG22	2.13	0.47
1:B:421:THR:HG23	1:B:421:THR:O	2.15	0.47
1:B:471:ILE:C	1:B:473:HIS:H	2.21	0.47
1:A:59:ALA:HB2	1:A:263:ILE:HD13	1.96	0.47
1:A:429:VAL:HG22	1:A:430:ALA:N	2.29	0.47
1:A:605:GLN:O	1:A:609:GLY:HA3	2.14	0.47
1:B:272:GLU:O	1:B:278:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASP:OD2	1:A:92:GLN:HG3	2.14	0.47
1:A:259:LYS:HE2	1:A:262:LEU:HD23	1.95	0.47
1:B:174:CYS:HB2	1:B:183:ASN:HD21	1.79	0.47
1:A:112:LEU:HD12	1:A:135:LEU:CD2	2.44	0.47
1:A:120:THR:HG21	1:A:188:TYR:CD1	2.50	0.47
1:A:388:ALA:O	1:A:389:MSE:HB3	2.14	0.47
1:A:471:ILE:O	1:A:473:HIS:ND1	2.47	0.47
1:B:84:PHE:C	1:B:85:TYR:CD1	2.92	0.47
1:B:117:SER:O	1:B:157:SER:CB	2.62	0.47
1:B:533:VAL:HB	1:B:537:THR:OG1	2.15	0.47
1:A:84:PHE:HB2	1:A:91:PRO:O	2.15	0.47
1:B:111:GLN:C	1:B:113:ARG:H	2.22	0.47
1:B:383:ASN:HD21	1:B:385:GLU:H	1.60	0.47
1:B:569:LYS:HD3	1:B:577:CYS:SG	2.55	0.47
1:A:23:ARG:HB2	1:A:37:VAL:O	2.15	0.47
1:A:133:GLY:HA2	1:A:326:LEU:HD13	1.97	0.47
1:A:460:TRP:O	1:A:463:PRO:HG2	2.14	0.47
1:A:462:ILE:HD13	1:A:580:ALA:HB3	1.97	0.47
1:B:548:ASP:HB3	1:B:549:PRO:HD2	1.96	0.47
1:A:201:ASP:OD2	1:A:201:ASP:N	2.47	0.47
1:A:414:LYS:HD2	1:A:414:LYS:O	2.15	0.47
1:B:267:LEU:O	1:B:302:PHE:HD2	1.98	0.47
1:B:342:VAL:HG23	1:B:600:ILE:HD12	1.96	0.47
1:A:632:ARG:NH2	2:A:9202:CIT:H42	2.30	0.47
1:B:130:ILE:HD11	1:B:319:TYR:HE1	1.80	0.47
1:A:460:TRP:HD1	1:A:461:ASN:HD22	1.63	0.47
1:A:510:ASN:C	1:A:512:GLU:H	2.21	0.47
1:B:407:VAL:HG12	1:B:594:GLU:HG3	1.97	0.47
1:B:398:ILE:HG12	1:B:671:LEU:HG	1.96	0.46
1:A:382:MSE:SE	1:A:402:CYS:HB3	2.65	0.46
1:A:518:THR:HG22	1:A:541:ASN:OD1	2.15	0.46
1:A:108:GLN:HB2	1:A:110:ASN:HD21	1.79	0.46
1:A:361:ASN:O	1:A:608:PHE:CZ	2.69	0.46
1:A:216:ASN:HB2	1:A:219:ASP:CG	2.40	0.46
1:A:643:ASP:O	1:A:645:ASN:N	2.43	0.46
1:A:646:THR:O	1:A:647:TYR:C	2.59	0.46
1:B:163:ASP:OD2	1:B:163:ASP:C	2.56	0.46
1:B:545:LYS:O	1:B:547:PRO:HD3	2.15	0.46
1:A:232:ARG:C	1:A:233:LYS:HG3	2.41	0.46
1:A:287:SER:HB2	1:A:290:GLY:O	2.16	0.46
1:A:439:LEU:HA	1:A:443:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:LEU:HD21	1:A:527:LYS:HB2	1.97	0.46
1:A:602:ARG:HH11	1:A:602:ARG:CB	2.09	0.46
1:A:627:LYS:O	1:A:628:ASP:C	2.59	0.46
1:B:27:LYS:HZ2	1:B:30:ILE:HD11	1.81	0.46
1:B:644:ARG:O	1:B:645:ASN:C	2.59	0.46
1:A:121:GLY:HA2	1:A:160:PRO:HD2	1.97	0.46
1:B:378:ILE:O	1:B:382:MSE:HG2	2.16	0.46
1:A:499:MSE:O	1:A:505:LEU:HD12	2.16	0.46
1:A:574:TYR:CD1	1:A:575:ALA:N	2.83	0.46
1:B:22:PHE:HA	1:B:282:PHE:CE2	2.51	0.46
1:B:489:LYS:H	1:B:489:LYS:HD3	1.81	0.46
1:A:538:VAL:HB	1:A:571:VAL:HG11	1.97	0.45
1:B:184:GLN:O	1:B:190:GLY:HA2	2.16	0.45
1:B:542:THR:HB	1:B:555:ASN:C	2.41	0.45
1:A:562:LEU:HD23	1:A:563:CYS:O	2.16	0.45
1:B:342:VAL:HB	1:B:366:ILE:CD1	2.45	0.45
1:A:83:GLU:CD	1:A:249:HIS:HD2	2.24	0.45
1:A:109:MSE:N	1:A:226:LEU:HD22	2.31	0.45
1:A:363:VAL:HG12	1:A:363:VAL:O	2.17	0.45
1:B:111:GLN:C	1:B:113:ARG:N	2.74	0.45
1:B:192:PHE:CZ	1:B:210:ILE:HG13	2.50	0.45
1:A:217:LYS:HA	1:A:220:ARG:HD2	1.98	0.45
1:A:524:LEU:C	1:A:526:GLU:H	2.22	0.45
1:A:283:GLN:N	1:A:283:GLN:OE1	2.49	0.45
1:B:418:CYS:HA	1:B:421:THR:HG22	1.97	0.45
1:B:98:VAL:HB	1:B:225:LEU:HG	1.98	0.45
1:B:394:GLY:O	1:B:397:TYR:HB3	2.17	0.45
1:A:120:THR:HG22	1:A:188:TYR:HA	1.98	0.45
1:A:374:THR:HG21	1:A:395:PHE:CD2	2.51	0.45
1:A:376:ASP:O	1:A:377:CYS:C	2.59	0.45
1:A:448:LYS:O	1:A:529:ASP:HB2	2.16	0.45
1:B:4:LYS:NZ	1:B:4:LYS:HB3	2.32	0.45
1:B:173:LEU:HG	1:B:199:ALA:HB1	1.98	0.45
1:B:344:TRP:CE2	1:B:389:MSE:HA	2.52	0.45
1:B:452:THR:HG22	1:B:517:TYR:HA	1.98	0.45
1:A:60:VAL:HG22	1:A:61:THR:H	1.82	0.45
1:A:177:CYS:O	1:A:178:GLY:C	2.60	0.45
1:A:192:PHE:CD1	1:A:213:ASN:HB2	2.52	0.45
1:A:407:VAL:HG23	1:A:408:LEU:N	2.31	0.45
1:B:64:ALA:HB2	1:B:246:VAL:CG2	2.46	0.45
1:A:293:LEU:C	1:A:295:PHE:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:ASN:HD22	1:B:645:ASN:HA	1.66	0.45
1:A:632:ARG:HB3	1:A:634:ASP:OD2	2.16	0.44
1:B:52:ILE:HA	1:B:57:ALA:O	2.17	0.44
1:B:600:ILE:O	1:B:603:GLN:HG2	2.17	0.44
1:A:338:GLU:O	1:A:339:CYS:HB2	2.16	0.44
1:A:417:ASN:N	1:A:417:ASN:OD1	2.50	0.44
1:A:477:ASP:C	1:A:479:PHE:H	2.26	0.44
1:A:535:HIS:HB2	1:A:574:TYR:CD2	2.51	0.44
1:B:336:THR:HB	1:B:337:ASP:H	1.44	0.44
1:B:451:HIS:HB3	1:B:459:GLY:O	2.17	0.44
1:B:475:ARG:N	1:B:475:ARG:CD	2.69	0.44
1:B:487:GLY:HA2	1:B:508:PRO:HD3	1.99	0.44
1:B:589:THR:HG21	1:B:597:VAL:HG21	1.99	0.44
1:A:191:ALA:O	1:A:194:CYS:HB3	2.17	0.44
1:A:60:VAL:HG22	1:A:61:THR:N	2.31	0.44
1:B:432:VAL:HG22	1:B:433:LYS:N	2.32	0.44
1:B:534:LYS:HE3	1:B:536:GLN:CG	2.48	0.44
1:A:81:VAL:HB	1:A:251:VAL:HB	1.98	0.44
1:A:192:PHE:HD1	1:A:213:ASN:HB2	1.83	0.44
1:A:615:CYS:O	1:A:616:SER:HB2	2.18	0.44
1:B:42:LYS:HE3	1:B:51:ALA:HB2	1.98	0.44
1:B:160:PRO:C	1:B:161:CYS:SG	3.00	0.44
1:B:591:LYS:HE2	1:B:591:LYS:HB2	1.79	0.44
1:A:75:ASN:O	1:A:76:ASN:C	2.60	0.44
1:A:276:LYS:C	1:A:278:LYS:H	2.26	0.44
1:A:552:LYS:HD3	1:A:553:ASN:H	1.82	0.44
1:A:671:LEU:HD22	1:A:671:LEU:O	2.17	0.44
1:B:405:VAL:CG1	1:B:591:LYS:HD3	2.47	0.44
1:A:406:PRO:O	1:A:641:LEU:HD12	2.18	0.44
1:A:429:VAL:HG23	1:A:577:CYS:O	2.17	0.44
1:B:26:MSE:HE2	1:B:266:LEU:HD12	1.98	0.44
1:B:71:TYR:HB2	1:B:311:ALA:CB	2.48	0.44
1:B:327:ARG:HH11	1:B:327:ARG:HG2	1.81	0.44
1:A:509:ASN:N	1:A:509:ASN:ND2	2.64	0.44
1:A:634:ASP:OD2	1:A:634:ASP:N	2.49	0.44
1:B:499:MSE:HG3	1:B:500:GLY:H	1.83	0.44
1:A:101:VAL:HG22	1:A:224:GLU:O	2.17	0.44
1:A:140:PRO:HG3	1:A:152:ASN:HB2	2.00	0.44
1:A:482:GLU:HA	1:A:493:SER:OG	2.17	0.44
1:A:602:ARG:NH1	1:A:602:ARG:CB	2.77	0.44
1:A:214:LEU:HA	1:A:214:LEU:HD12	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:PRO:HD3	1:A:571:VAL:HG11	2.00	0.43
1:B:85:TYR:CD1	1:B:85:TYR:N	2.85	0.43
1:B:91:PRO:HG2	1:B:92:GLN:H	1.82	0.43
1:B:389:MSE:HE2	1:B:391:LEU:CD2	2.47	0.43
1:A:194:CYS:O	1:A:199:ALA:HB3	2.18	0.43
1:A:268:ASN:O	1:A:271:GLN:HG2	2.19	0.43
1:A:309:MSE:HE1	1:A:677:ARG:HG3	2.00	0.43
1:B:31:PRO:C	1:B:33:ASP:H	2.26	0.43
1:B:134:LEU:HG	1:B:322:ALA:HB2	1.99	0.43
1:A:110:ASN:HD22	1:A:110:ASN:H	1.64	0.43
1:A:110:ASN:HB3	1:A:230:ASN:OD1	2.18	0.43
1:A:316:GLY:O	1:A:320:VAL:HG23	2.17	0.43
1:A:351:GLU:HG2	1:A:630:LEU:HD21	1.93	0.43
1:A:365:LYS:HE2	1:A:603:GLN:HE22	1.84	0.43
1:B:29:VAL:CB	1:B:273:HIS:ND1	2.76	0.43
1:B:103:LYS:HA	1:B:224:GLU:CD	2.43	0.43
1:B:371:ALA:HB3	1:B:377:CYS:SG	2.58	0.43
1:B:534:LYS:HE3	1:B:536:GLN:CD	2.44	0.43
1:A:308:ARG:HB2	1:A:669:SER:CB	2.43	0.43
1:A:23:ARG:CA	1:A:37:VAL:HG13	2.39	0.43
1:A:268:ASN:C	1:A:270:ALA:N	2.74	0.43
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.88	0.43
1:A:26:MSE:C	1:A:28:SER:H	2.26	0.43
1:B:79:PRO:HB3	1:B:250:THR:HG21	1.99	0.43
1:B:127:GLY:HA2	1:B:204:PHE:O	2.19	0.43
1:B:462:ILE:N	1:B:463:PRO:HD2	2.34	0.43
1:A:128:TRP:C	1:A:131:PRO:HD2	2.43	0.43
1:A:381:ILE:O	1:A:381:ILE:HG22	2.19	0.43
1:A:440:THR:CG2	1:A:441:TRP:N	2.81	0.43
1:A:592:ASP:O	1:A:593:LYS:HB2	2.19	0.43
1:B:400:GLY:HA3	1:B:647:TYR:CD2	2.54	0.43
1:A:85:TYR:HD1	1:A:298:SER:O	2.01	0.43
1:B:355:CYS:HA	1:B:630:LEU:HD11	2.00	0.43
1:B:407:VAL:O	1:B:408:LEU:HG	2.18	0.43
1:A:113:ARG:HG2	1:A:113:ARG:NH1	2.33	0.43
1:A:274:PHE:HB3	1:A:282:PHE:O	2.18	0.43
1:A:544:GLY:HA2	1:A:553:ASN:HA	2.01	0.43
1:A:591:LYS:HD2	1:A:591:LYS:O	2.18	0.43
1:A:15:GLU:HA	1:A:293:LEU:HD23	2.00	0.43
1:A:26:MSE:C	1:A:28:SER:N	2.77	0.43
1:A:647:TYR:O	1:A:651:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:VAL:HG11	1:B:45:TYR:CD1	2.53	0.43
1:B:535:HIS:HB2	1:B:574:TYR:CD2	2.54	0.43
1:B:640:LYS:CB	1:B:644:ARG:HH12	2.32	0.43
1:A:618:ASN:HD22	1:A:618:ASN:HA	1.58	0.42
1:B:225:LEU:HD13	1:B:235:VAL:HG12	2.00	0.42
1:B:392:ASP:O	1:B:393:GLY:C	2.63	0.42
1:A:107:PHE:CE2	1:A:226:LEU:HD11	2.53	0.42
1:A:224:GLU:HA	1:A:235:VAL:HG13	2.00	0.42
1:B:172:GLN:O	1:B:172:GLN:HG2	2.20	0.42
1:B:535:HIS:HB2	1:B:574:TYR:CG	2.53	0.42
1:A:266:LEU:HD23	1:A:267:LEU:CA	2.48	0.42
1:A:490:LYS:HA	1:A:495:CYS:SG	2.60	0.42
1:B:663:ARG:HD3	1:B:663:ARG:HA	1.79	0.42
1:A:87:SER:C	1:A:89:GLU:H	2.27	0.42
1:A:91:PRO:O	1:A:92:GLN:HB2	2.20	0.42
1:A:243:LEU:N	1:A:243:LEU:HD12	2.35	0.42
1:B:27:LYS:HE3	1:B:27:LYS:CA	2.43	0.42
1:B:489:LYS:HG2	1:B:492:SER:HB2	2.00	0.42
1:B:108:GLN:HA	1:B:108:GLN:HE21	1.84	0.42
1:B:483:GLY:HA2	1:B:497:LEU:CD1	2.48	0.42
1:A:653:GLU:O	1:A:656:VAL:HG22	2.20	0.42
1:B:546:ASN:ND2	1:B:548:ASP:HB2	2.34	0.42
1:A:35:PRO:HB2	1:A:266:LEU:HB2	2.02	0.42
1:A:254:ARG:HB2	1:A:258:GLY:HA2	2.01	0.42
1:A:462:ILE:CG2	1:A:580:ALA:HB3	2.50	0.42
1:A:610:SER:HB2	1:A:636:VAL:O	2.20	0.42
1:B:258:GLY:O	1:B:259:LYS:HB2	2.18	0.42
1:B:341:PRO:HB3	1:B:367:GLU:HG3	2.02	0.42
1:A:110:ASN:ND2	1:A:111:GLN:HG2	2.35	0.42
1:A:391:LEU:HD13	1:A:395:PHE:HB3	2.02	0.42
1:A:524:LEU:C	1:A:526:GLU:N	2.78	0.42
1:A:538:VAL:C	1:A:540:GLN:H	2.27	0.42
1:A:551:ALA:O	1:A:552:LYS:C	2.62	0.42
1:A:562:LEU:C	1:A:577:CYS:SG	3.03	0.42
1:A:651:LEU:HD12	1:A:656:VAL:HG12	2.02	0.42
1:B:383:ASN:ND2	1:B:385:GLU:N	2.62	0.42
1:B:412:TYR:HA	1:B:636:VAL:HG23	2.01	0.42
1:B:485:ALA:O	1:B:486:PRO:C	2.62	0.42
1:B:641:LEU:HG	1:B:644:ARG:HD3	2.02	0.42
1:A:335:PRO:C	1:A:337:ASP:H	2.28	0.42
1:A:371:ALA:HB3	1:A:377:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:MSE:HB2	1:A:500:GLY:H	1.56	0.42
1:B:344:TRP:O	1:B:369:VAL:HG12	2.20	0.42
1:B:485:ALA:HB3	1:B:494:LEU:HB3	2.01	0.42
1:A:391:LEU:HB3	1:A:395:PHE:HB2	2.02	0.41
1:A:412:TYR:CE1	1:A:632:ARG:NH1	2.88	0.41
1:B:148:LYS:HB2	1:B:167:PHE:HE1	1.85	0.41
1:B:214:LEU:HD11	1:B:223:TYR:CE2	2.54	0.41
1:A:71:TYR:HB2	1:A:311:ALA:CB	2.50	0.41
1:A:309:MSE:SE	1:A:314:TYR:HD1	2.53	0.41
1:A:483:GLY:CA	1:A:497:LEU:HD13	2.50	0.41
1:A:510:ASN:C	1:A:512:GLU:N	2.78	0.41
1:B:14:HIS:HB3	1:B:293:LEU:HD21	2.02	0.41
1:B:499:MSE:CG	1:B:500:GLY:H	2.33	0.41
1:A:381:ILE:HA	1:A:386:ALA:O	2.20	0.41
1:B:400:GLY:C	1:B:402:CYS:N	2.78	0.41
1:A:22:PHE:CE1	1:A:284:LEU:HD13	2.56	0.41
1:A:25:HIS:NE2	1:A:282:PHE:HB2	2.35	0.41
1:B:569:LYS:HB3	1:B:573:GLU:OE1	2.20	0.41
1:A:171:CYS:O	1:A:175:PRO:N	2.53	0.41
1:A:254:ARG:HB2	1:A:258:GLY:CA	2.50	0.41
1:A:342:VAL:HG23	1:A:600:ILE:CD1	2.42	0.41
1:B:26:MSE:C	1:B:28:SER:H	2.29	0.41
1:B:192:PHE:O	1:B:195:LEU:HB3	2.21	0.41
1:B:308:ARG:HA	1:B:308:ARG:HD2	1.75	0.41
1:A:19:CYS:C	1:A:39:CYS:SG	3.04	0.41
1:A:534:LYS:NZ	1:A:536:GLN:HE21	2.19	0.41
1:B:83:GLU:OE1	1:B:299:ALA:HB2	2.20	0.41
1:A:428:ALA:O	1:A:579:LEU:HB2	2.20	0.41
1:A:552:LYS:HG2	1:A:553:ASN:N	2.36	0.41
1:A:374:THR:HG21	1:A:395:PHE:CG	2.55	0.41
1:B:188:TYR:HD1	1:B:205:VAL:HB	1.86	0.41
1:B:574:TYR:CD1	1:B:575:ALA:N	2.89	0.41
1:A:248:SER:O	1:A:249:HIS:HB2	2.21	0.41
1:A:342:VAL:HB	1:A:366:ILE:HD13	2.02	0.41
1:A:399:ALA:HB1	1:A:404:LEU:HD12	2.02	0.41
1:A:524:LEU:HB2	1:A:531:ALA:HB2	2.02	0.41
1:A:621:LEU:HD21	1:A:631:PHE:HE2	1.86	0.41
1:B:217:LYS:HD3	1:B:221:ASP:OD2	2.20	0.41
1:B:381:ILE:HB	1:B:404:LEU:HD21	2.02	0.41
1:B:456:ARG:O	1:B:460:TRP:HB3	2.21	0.41
1:B:603:GLN:O	1:B:606:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:CYS:HB3	1:A:389:MSE:SE	2.71	0.41
1:A:454:VAL:O	1:A:454:VAL:HG23	2.21	0.41
1:A:514:TYR:OH	1:A:526:GLU:OE1	2.33	0.41
1:B:210:ILE:HG23	1:B:211:PHE:N	2.36	0.41
1:B:90:ASP:OD2	1:B:92:GLN:HG3	2.21	0.40
1:B:128:TRP:O	1:B:132:ILE:HB	2.21	0.40
1:B:431:VAL:HG13	1:B:524:LEU:CD2	2.51	0.40
1:B:8:TRP:CH2	1:B:267:LEU:HD11	2.55	0.40
1:B:392:ASP:OD2	1:B:392:ASP:C	2.65	0.40
1:B:437:SER:HA	1:B:568:ARG:HH12	1.86	0.40
1:A:37:VAL:HG13	1:A:37:VAL:O	2.20	0.40
1:A:266:LEU:HD23	1:A:266:LEU:C	2.45	0.40
1:A:597:VAL:O	1:A:601:LEU:HB2	2.22	0.40
1:B:291:LYS:HD2	1:B:291:LYS:HA	1.83	0.40
1:B:292:ASP:HA	1:B:295:PHE:O	2.21	0.40
1:B:589:THR:OG1	1:B:590:ARG:N	2.55	0.40
1:B:657:LYS:HE3	1:B:657:LYS:HB2	1.90	0.40
1:A:440:THR:CG2	1:A:441:TRP:H	2.31	0.40
1:B:533:VAL:HG11	1:B:537:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	674/676 (100%)	566 (84%)	89 (13%)	19 (3%)	4	9
1	B	674/676 (100%)	572 (85%)	80 (12%)	22 (3%)	3	7
All	All	1348/1352 (100%)	1138 (84%)	169 (12%)	41 (3%)	3	8

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	PRO
1	A	501	SER
1	A	628	ASP
1	B	162	ALA
1	B	338	GLU
1	B	435	SER
1	A	278	LYS
1	A	453	ALA
1	A	499	MSE
1	A	553	ASN
1	A	629	LEU
1	B	125	SER
1	B	178	GLY
1	B	332	PRO
1	B	436	ALA
1	B	471	ILE
1	B	629	LEU
1	A	417	ASN
1	A	472	ASN
1	A	567	THR
1	A	644	ARG
1	B	469	ASN
1	B	549	PRO
1	B	552	LYS
1	B	567	THR
1	B	628	ASP
1	A	329	GLY
1	A	438	ASP
1	A	593	LYS
1	B	163	ASP
1	B	445	LYS
1	B	472	ASN
1	A	527	LYS
1	B	416	ASP
1	B	460	TRP
1	A	420	ASP
1	A	577	CYS
1	B	277	ASP
1	B	486	PRO
1	B	533	VAL
1	A	549	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	569/560 (102%)	526 (92%)	43 (8%)	12	30
1	B	569/560 (102%)	519 (91%)	50 (9%)	9	23
All	All	1138/1120 (102%)	1045 (92%)	93 (8%)	10	27

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	32	SER
1	A	33	ASP
1	A	67	VAL
1	A	110	ASN
1	A	184	GLN
1	A	201	ASP
1	A	214	LEU
1	A	225	LEU
1	A	226	LEU
1	A	228	LEU
1	A	246	VAL
1	A	266	LEU
1	A	278	LYS
1	A	283	GLN
1	A	291	LYS
1	A	304	LYS
1	A	326	LEU
1	A	338	GLU
1	A	347	LEU
1	A	348	SER
1	A	351	GLU
1	A	444	LEU
1	A	445	LYS
1	A	473	HIS
1	A	495	CYS
1	A	499	MSE

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Mol	Chain	Res	Type
1	A	509	ASN
1	A	511	LYS
1	A	533	VAL
1	A	541	ASN
1	A	545	LYS
1	A	557	LYS
1	A	573	GLU
1	A	601	LEU
1	A	602	ARG
1	A	618	ASN
1	A	628	ASP
1	A	632	ARG
1	A	646	THR
1	A	654	GLU
1	A	670	LEU
1	A	678	ARG
1	B	4	LYS
1	B	13	GLU
1	B	21	SER
1	B	27	LYS
1	B	41	LYS
1	B	46	LEU
1	B	74	PRO
1	B	93	THR
1	B	122	LEU
1	B	125	SER
1	B	181	THR
1	B	193	LYS
1	B	225	LEU
1	B	233	LYS
1	B	239	LYS
1	B	240	ASP
1	B	246	VAL
1	B	280	LYS
1	B	281	GLU
1	B	326	LEU
1	B	336	THR
1	B	339	CYS
1	B	374	THR
1	B	383	ASN
1	B	389	MSE
1	B	420	ASP

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Mol	Chain	Res	Type
1	B	423	GLU
1	B	434	LYS
1	B	473	HIS
1	B	475	ARG
1	B	489	LYS
1	B	509	ASN
1	B	525	VAL
1	B	527	LYS
1	B	538	VAL
1	B	552	LYS
1	B	558	ASP
1	B	573	GLU
1	B	591	LYS
1	B	604	GLN
1	B	613	THR
1	B	623	ARG
1	B	624	SER
1	B	641	LEU
1	B	644	ARG
1	B	645	ASN
1	B	646	THR
1	B	654	GLU
1	B	662	LEU
1	B	671	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	76	ASN
1	A	110	ASN
1	A	152	ASN
1	A	213	ASN
1	A	245	GLN
1	A	249	HIS
1	A	273	HIS
1	A	361	ASN
1	A	411	ASN
1	A	451	HIS
1	A	461	ASN
1	A	509	ASN
1	A	510	ASN

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Mol	Chain	Res	Type
1	A	535	HIS
1	A	536	GLN
1	A	546	ASN
1	A	576	ASN
1	A	578	HIS
1	A	603	GLN
1	A	606	HIS
1	A	618	ASN
1	A	642	HIS
1	A	645	ASN
1	B	20	GLN
1	B	55	ASN
1	B	108	GLN
1	B	111	GLN
1	B	183	ASN
1	B	245	GLN
1	B	249	HIS
1	B	271	GLN
1	B	325	ASN
1	B	361	ASN
1	B	383	ASN
1	B	417	ASN
1	B	451	HIS
1	B	509	ASN
1	B	535	HIS
1	B	536	GLN
1	B	546	ASN
1	B	642	HIS
1	B	645	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CIT	B	9204	-	12,12,12	1.95	2 (16%)	17,17,17	1.73	4 (23%)
3	GOL	A	9101	-	5,5,5	0.28	0	5,5,5	0.26	0
2	CIT	A	9202	-	12,12,12	1.88	2 (16%)	17,17,17	1.68	3 (17%)
3	GOL	B	9102	-	5,5,5	0.49	0	5,5,5	0.32	0
2	CIT	B	9201	-	12,12,12	1.93	2 (16%)	17,17,17	1.69	3 (17%)
2	CIT	B	9206	-	12,12,12	1.96	2 (16%)	17,17,17	1.72	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	B	9204	-	-	2/16/16/16	-
3	GOL	A	9101	-	-	0/4/4/4	-
2	CIT	A	9202	-	-	2/16/16/16	-
3	GOL	B	9102	-	-	0/4/4/4	-
2	CIT	B	9201	-	-	2/16/16/16	-
2	CIT	B	9206	-	-	2/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9204	CIT	C2-C3	5.05	1.60	1.54
2	B	9201	CIT	C2-C3	4.70	1.59	1.54
2	B	9206	CIT	C2-C3	4.64	1.59	1.54
2	A	9202	CIT	C2-C3	4.15	1.59	1.54
2	B	9206	CIT	C4-C3	3.63	1.58	1.54
2	A	9202	CIT	C4-C3	3.52	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9201	CIT	C4-C3	3.17	1.57	1.54
2	B	9204	CIT	C4-C3	2.92	1.57	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9201	CIT	O6-C6-O5	-3.75	111.87	123.86
2	A	9202	CIT	O6-C6-O5	-3.74	111.89	123.86
2	B	9204	CIT	O6-C6-O5	-3.54	112.54	123.86
2	B	9206	CIT	O6-C6-O5	-3.49	112.70	123.86
2	B	9204	CIT	O5-C6-C3	-2.98	116.32	122.09
2	B	9206	CIT	O5-C6-C3	-2.90	116.47	122.09
2	B	9201	CIT	O5-C6-C3	-2.54	117.17	122.09
2	B	9204	CIT	C4-C3-C6	-2.53	104.43	110.03
2	A	9202	CIT	O5-C6-C3	-2.48	117.28	122.09
2	B	9206	CIT	C4-C3-C6	-2.12	105.34	110.03
2	B	9201	CIT	O4-C5-C4	2.06	120.86	114.35
2	A	9202	CIT	O4-C5-C4	2.03	120.78	114.35
2	B	9204	CIT	O7-C3-C2	2.02	113.99	109.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9202	CIT	C2-C3-C6-O5
2	A	9202	CIT	O7-C3-C6-O5
2	B	9201	CIT	C2-C3-C6-O5
2	B	9201	CIT	O7-C3-C6-O5
2	B	9204	CIT	C2-C3-C6-O5
2	B	9204	CIT	O7-C3-C6-O5
2	B	9206	CIT	C2-C3-C6-O5
2	B	9206	CIT	O7-C3-C6-O5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9202	CIT	1	0
2	B	9206	CIT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	667/676 (98%)	0.76	69 (10%)	12 10	27, 66, 113, 122	0
1	B	667/676 (98%)	0.57	35 (5%)	33 29	26, 62, 102, 113	0
All	All	1334/1352 (98%)	0.66	104 (7%)	19 16	26, 64, 108, 122	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	483	GLY	4.6
1	A	514	TYR	4.0
1	A	484	CYS	3.8
1	A	570	PRO	3.7
1	A	29	VAL	3.6
1	A	486	PRO	3.6
1	B	612	VAL	3.6
1	A	497	LEU	3.6
1	A	284	LEU	3.4
1	B	639	ALA	3.4
1	A	515	TYR	3.3
1	A	550	TRP	3.3
1	B	644	ARG	3.3
1	B	561	LEU	3.3
1	A	439	LEU	3.2
1	A	289	HIS	3.2
1	B	641	LEU	3.2
1	B	210	ILE	3.2
1	A	513	GLY	3.1
1	A	493	SER	3.1
1	A	22	PHE	3.0
1	B	645	ASN	3.0
1	A	612	VAL	2.9
1	A	274	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	564	LEU	2.9
1	A	286	SER	2.9
1	B	472	ASN	2.9
1	A	495	CYS	2.9
1	A	485	ALA	2.8
1	B	199	ALA	2.8
1	A	579	LEU	2.8
1	A	559	TYR	2.7
1	B	562	LEU	2.7
1	A	571	VAL	2.7
1	B	185	TYR	2.7
1	A	498	CYS	2.6
1	A	520	ALA	2.6
1	A	36	SER	2.5
1	B	273	HIS	2.5
1	A	282	PHE	2.5
1	A	226	LEU	2.5
1	B	439	LEU	2.5
1	A	577	CYS	2.5
1	A	28	SER	2.5
1	A	521	PHE	2.5
1	A	418	CYS	2.5
1	B	541	ASN	2.4
1	A	438	ASP	2.4
1	A	566	GLY	2.4
1	A	490	LYS	2.4
1	A	336	THR	2.4
1	B	107	PHE	2.4
1	A	13	GLU	2.4
1	B	160	PRO	2.4
1	A	436	ALA	2.4
1	A	177	CYS	2.3
1	B	121	GLY	2.3
1	A	551	ALA	2.3
1	A	562	LEU	2.3
1	A	443	ASN	2.3
1	A	541	ASN	2.3
1	B	549	PRO	2.3
1	B	547	PRO	2.3
1	A	107	PHE	2.3
1	B	159	ALA	2.3
1	A	452	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	528	GLY	2.3
1	A	494	LEU	2.3
1	B	25	HIS	2.2
1	B	613	THR	2.2
1	A	169	GLN	2.2
1	A	170	LEU	2.2
1	A	267	LEU	2.2
1	B	29	VAL	2.2
1	A	642	HIS	2.2
1	A	449	SER	2.2
1	A	192	PHE	2.2
1	B	471	ILE	2.2
1	A	421	THR	2.2
1	B	200	GLY	2.2
1	A	100	VAL	2.2
1	B	335	PRO	2.1
1	B	494	LEU	2.1
1	A	543	GLY	2.1
1	B	186	PHE	2.1
1	B	486	PRO	2.1
1	A	225	LEU	2.1
1	A	505	LEU	2.1
1	A	516	GLY	2.1
1	B	559	TYR	2.1
1	A	63	ASP	2.1
1	A	643	ASP	2.1
1	A	149	ALA	2.1
1	B	646	THR	2.1
1	A	275	GLY	2.1
1	A	450	CYS	2.1
1	A	473	HIS	2.1
1	B	544	GLY	2.1
1	A	53	ALA	2.0
1	B	269	GLN	2.0
1	B	443	ASN	2.0
1	A	517	TYR	2.0
1	A	563	CYS	2.0
1	A	180	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	B	9201	13/13	0.44	0.19	98,101,103,104	0
3	GOL	B	9102	6/6	0.57	0.17	93,97,97,97	0
3	GOL	A	9101	6/6	0.58	0.22	101,101,101,102	0
2	CIT	A	9202	13/13	0.67	0.18	104,106,107,107	0
2	CIT	B	9204	13/13	0.69	0.16	111,112,115,115	0
2	CIT	B	9206	13/13	0.70	0.16	115,116,116,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.